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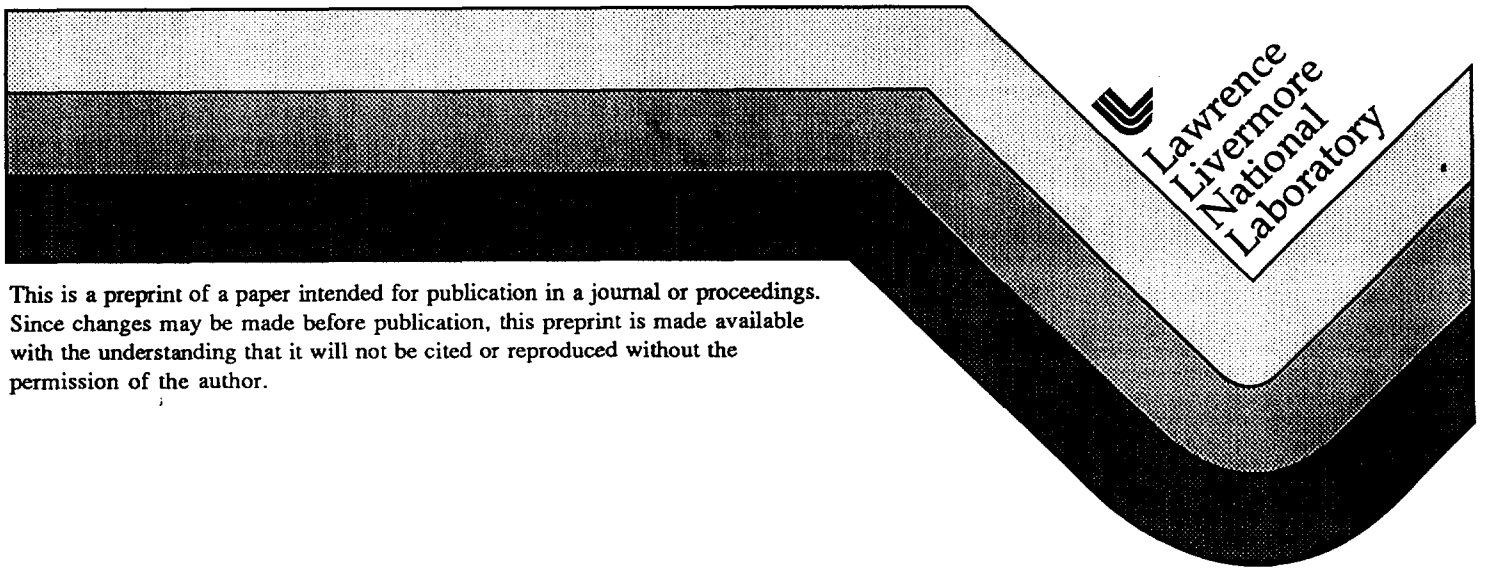

Simple Numerical Models for Antiproton-Hydrogen Scattering

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Abstract

A large difference exists between two calculations of the antiproton capture cross section in antiproton - hydrogen atom scattering for antiproton energies around 1 meV. One of these, a semiclassical calculation more likely to be valid at higher energies, is incapable of a detailed description of the quantum processes that occur when the particles are separated by distances of about one Bohr radius. The other calculation, fully quantum mechanical and valid below 1 meV, shows that these details can lower the cross section considerably. A fully quantum mechanical calculation at the higher energies is extremely difficult, but solvable model problems can be formulated to help determine the validity of the semiclassical results.

1. Introduction

There have been a number of calculations of the antiproton (p^-) - hydrogen atom (H) scattering interaction for incident p^- energies around and below about 30 eV (lab frame) where the p^- can easily be captured by the proton (p) of H to form protonium (Pn) while the e^- of H escapes. Morgan and Hughes employed a semiclassical approximation valid from possibly 1 meV to about 10 eV to obtain the Pn formation cross section (σ) [1-4]. Assuming the p^- motion is classical, Morgan translated the results of others, who used various methods for the scattering of negative muons by H, into σ for p^--H scattering [2]. This was done from 3 eV to somewhat beyond 25 eV where σ decreases rapidly. Voronin and Carbonell have calculated p^--H scattering for energies from zero to nearly 1 meV using an apparently accurate, fully quantum mechanical method [5].

While there is good agreement between Morgan's semiclassical and translated values [3], there is a large discrepancy between those of Morgan and Voronin. These both give an approximate $1/v$ ($v = p^-$ velocity) dependence for σ, but Voronin's values are two or three orders of magnitude lower. Even assuming there may be some invalidity in either around 1 meV, it is important to examine the calculations, in particular Morgan's semiclassical method which is very probably the more approximate of the two.

The semiclassical method treats the p^--p motion as classical and employs the adiabatic (Born-Oppenheimer) approximation to determine the quantum mechanical motion of the e^-. After the e^- energy in H has risen to nearly zero and the adiabatic approximation breaks down at a p^--p distance of about 1 a_0 (Bohr radius), it is assumed that the e^- absorbs a small amount of additional energy and becomes free, leaving the p and p^- in a bound state of Pn. However, at least at very low energies, Voronin finds a strong tendency for reversion to the initial state as the Pn is being formed (inverse Auger process), thus accounting for his very low σ's. This process could be present at higher energies, although Morgan has estimated that it lowers σ by only 20% [4]. It is conceivable that this estimate is in error because the semiclassical method neglects the discretness of Pn energies. At an initial p^- energy of zero the e^- must leave with a 0.28 eV energy in order that the Pn be left in the nearest discrete state (n=30). That energy decreases linearly to zero for an incident, lab-frame energy of 1.2 eV. Depending on how one estimates the kinetic energies of the p and p^- at the time of adiabatic breakdown, an energy of 0.28 eV is at least several times the maximum that can be transferred from either of these two particles to the e^- in a binary encounter. Thus it is only the details of the breakdown that might allow the e^- to absorb sufficient energy for Pn formation below 1 eV, and the semiclassical method does not, of course, provide those details.

An accurate, fully quantum mechanical calculation for energies from 1 meV to 1 eV could resolve this problem, but the large number of angular momentum waves that are likely to be relevant would make the problem intractable, even on supercomputers. Thus, I am seeking model problems which embody the same essential physics as is involved in the real p^--p-e^- system and whose solution would deal with the above issues. My intent is to begin with models involving only one equation of no more than 2 variables, which can be solved by numerical techniques and work up to more complicated models that more closely approximate the real problem. Two initial models and a short discussion of the means to solve them are described in the following sections.

2. Two Simple Models

The first step in formulating simple models is to give the p an infinite mass and the p^- a mass equal to half of that which it and the p share (i.e. give it the p^--p reduced mass). This is done to avoid cross derivative terms in the Schroedinger equation when the p^--p separation, **R**, and the e^--p separation, **r**, are used as the basis for a coordinate system. Such masses leave Pn states unaltered while altering the H ground state and the p^--H interaction only slightly. The e^--Pn interaction is altered to the extent that the e^- now experiences one moving particle that has twice the velocity had by each of the two with which it really interacts. It is likely that energy transfer will be sufficiently similar in this model to that in reality so that its use is valid.

The next step is to set the angular momentum of all particles to zero. Doing so would only alter Voronin's results a little, since the higher angular momenta contribute only a small amount to σ [5]. Such angular momenta contribute only 3% of the semiclassical σ at 1 meV, but that amount is still much greater than Voronin's full σ, so the discrepancy still exists with pure S states.

A further step in simplification is the choice of an appropriate potential energy. Two such possible choices, including the above simplifications, are shown in Fig. 1. The "square well" model for the potential energy was chosen in the hope that its mathematics would be simple enough for an analytic solution to be possible. It now appears that a numerical solution is necessary. The "split coulomb" model was chosen because its potential energy is that resulting from averaging the p^--e^- potential energy over the angle between these two particles. Both render the Schroedinger equation separable inside each potential energy region. If we take

$$\psi = (1/rR)\,\chi \quad \text{and} \quad \chi = \Sigma_j\, \chi_{Pj}[R]\, \chi_{ej}[r] \ , \tag{1}$$

where Σ_j might be wholly or in part an integral, then the Schroedinger equation gives (using electron atomic units):

$$((1/m)d^2/dR^2 + 2E_{Pj})\,\chi_{Pj} = 0 \quad \text{and} \quad (d^2/dr^2 + 2E_{ej})\,\chi_{ej} = 0 \ , \tag{2}$$

where E_{Pj} and E_{ej} are constants within each potential energy region of the square well model such that

$$E_{Pj} + E_{ej} = -V + E \ , \tag{3}$$

where the total energy, E, has the value

$$E = -1/2 + p^2/2m \ , \tag{4}$$

where -1/2 is the ground state energy of H in the model and p is the initial momentum of the reduced mass p^-. For the split coulomb model, Eq. (1) and (2) likewise apply, but here E_{Pj} and E_{ej} are not always constants, being given by

$$E_{Pj} = 1/R + E_{Pj}' \text{ (for } r > R), \quad = E_{Pj}' \text{ (for } r < R)$$

$$\text{and} \quad E_{ej} = 1/r + E_{ej}' \text{ (for } r < R), \quad = E_{ej}' \text{ (for } r > R) \ , \tag{5}$$

where E_{Pj}' and E_{ej}' are constants within each potential energy region and

$$E_{Pj}' + E_{ej}' = E \ , \tag{6}$$

where E is the same as in Eq. (4).

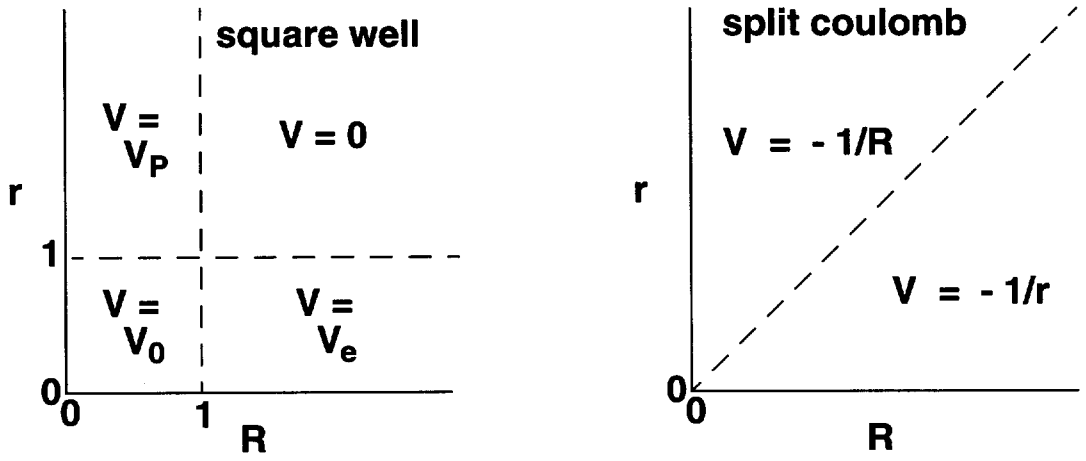

Figure 1. Potential energy assignments for the various regions in the simple models for p^--H scattering. Electron atomic units are employed.

The boundary conditions on χ of Eq. (1) are that it must be zero along R = 0 and r = 0 and that it must have the correct asymptotic forms:

$$\text{for } R \to \infty, \qquad \chi \to \chi_H[r]\,(c_+ e^{ipR} + c_- e^{-ipR}) \tag{7}$$

$$\text{and for } r \to \infty, \qquad \chi \to \Sigma_n\, c_n\, \chi_{bPn}[R]\, e^{ik[n]r} \ , \tag{8}$$

where $\chi_H[r]$ is r times the wave function for the H ground state in either model with energy -1/2 and $\chi_{bPn}[R]$ is R times the wave function for the n^{th} bound state of Pn in either model with energy, E_{bPn}. k depends on n according to:

$$(1/2)\, k^2 + E_{bPn} = E \ . \tag{9}$$

The second term in parentheses in Eq. (7) is the incoming p^- wave and the first term is the outgoing elastically scattered p^- wave. The exponential terms in Eq. (8) are outgoing e^- waves. The coefficients in these equations are determined by the solution of the problem for all R and r. In the split potential model, χ_H and χ_{bPn} represent the normal bound states of H and Pn for an infinite mass p, a half mass p^-, and a normal mass e^-. In the square well model, they are square-well bound states. V_e is chosen so that the energy of the H ground state is -1/2, which turns out to be the only bound state. To preserve the symmetry that exists in reality, V_p is taken equal to V_e in which case Pn has many bound states due to the large ratio of the p^- mass to that of the e^-.

In the steady state solution we seek for the Schroedinger equation, antiprotons enter from R = ∞, while electrons leave toward r = ∞. This conversion of antiprotons to electrons can occur because an E_{Pj} in Eq. (2) can have a negative imaginary part leading to antiproton destruction,

while the corresponding E_{ej} has a positive imaginary part of equal magnitude leading to electron creation. In Eq. (3) or (6), these parts cancel, leaving E real.

While the split coulomb model represents the asymptotic conditions nearly exactly, the square well model does not. Additionally, the square well model does not have the correct spacing between its Pn energy levels and may produce reflections at its region boundaries that are too large due to the potential energy discontinuities. On the other hand, that model involves only elementary transcendental functions.

3. Methods of Solution

Two basic methods of solution will be investigated. In the first, general solutions that satisfy the relevant boundary and asymptotic conditions are obtained for each region. Solution is then obtained by numerically solving the conditions on continuity of value and derivative of the wave function across each of the region boundaries. This is likely to involve discretization of these boundaries and, perhaps, those coefficients appearing in the general solutions that are continuous functions of their arguments (i.e. where one has integrals instead of sums). The second method is to numerically integrate the two-variable Schroedinger equation. While this may seem simpler, implicit methods may involve matrices that are too large, and explicit methods may require iteration back and forth between $R = \infty$ and $r = \infty$ to rid solutions of exponential functions that increase in these limits.

4. A Trial Problem

An even simpler problem results if one replaces the incident p^- with an e^- with spin opposite to that of the e^- in the H. An analytic solution will be attempted for this simpler problem as a means to test the numerical methods for solving the p^- problem.

5. Acknowledgment

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